Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Structural and dynamic characteristics of copper(II) amino acid complexes in solutions by combined EPR and NMR relaxation methods

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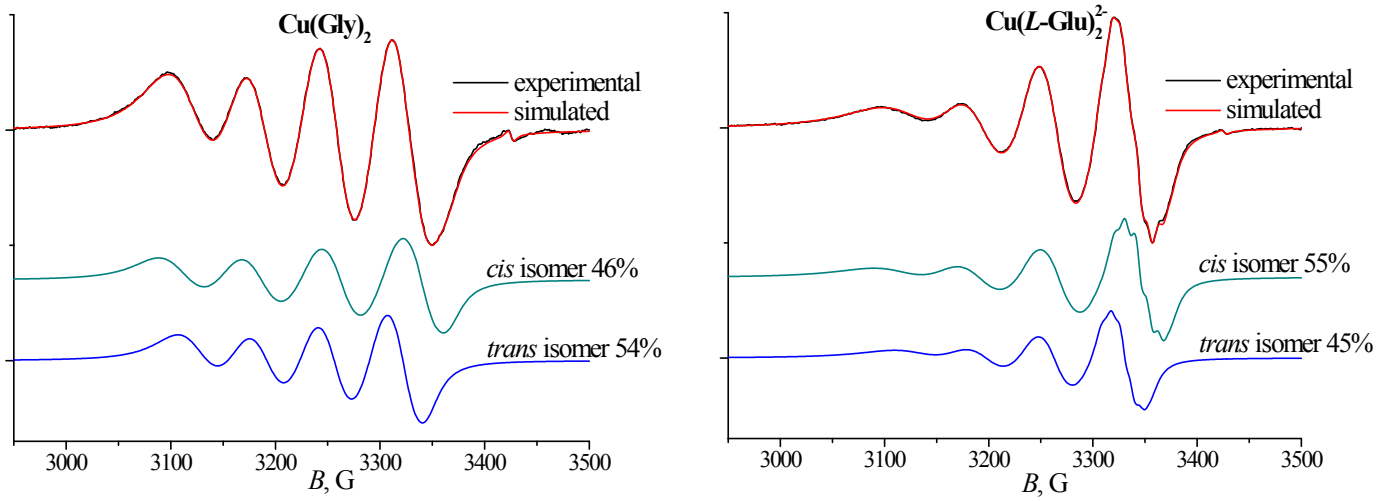

Fig. 1S Experimental and simulated EPR spectra of the $Cu(Gly)_2$ and $Cu(L\text{-}Glu)_2^{2-}$ complexes.

Table 1S EPR spectra parameters of the copper(II) complexes with amino acids at 295 (1.0 M KNO_3)

Complex	$g_\perp$	$g_\parallel$	g_0	$A_\perp$ / G	$A_\parallel$ / G	A_0 / G	$\tau_R \cdot 10^{11}$ / s	A_0^N / G	P 1.0 M KNO_3
$Cu(Gly)_2$									
trans isomer	2.052	2.267	2.1285	15	160	63.4	3.4	8.9	0.54
cis isomer	2.052	2.267	2.1277	20	180	74.2	3.4	10.5	0.46
$Cu(D\text{-}Ala)_2$									
trans isomer	2.052	2.257	2.1252	15	167	64.2	4.2	8.9	0.45
cis isomer	2.052	2.257	2.1240	20	180	75.0	4.2	10.5	0.55
$Cu(D\text{-}Val)_2$									
trans isomer	2.055	2.257	2.1223	15	163	64.5	5.2	8.6	0.51
cis isomer	2.055	2.255	2.1207	20	183	74.4	5.2	10.3	0.49
$Cu(L\text{-}Ser)_2$									
trans isomer	2.057	2.266	2.1262	15	167	64.3	4.8	8.9	0.51
cis isomer	2.057	2.266	2.1262	20	187	75.5	4.8	10.5	0.49
$Cu(L\text{-}Asp)_2^{2-}$									
trans isomer	2.065	2.2481	2.1260	15	144	57.9	6.2	9.4	0.40
cis isomer	2.065	2.2483	2.1261	20	174	71.5	6.2	10.2	0.60
$Cu(L\text{-}Glu)_2^{2-}$									
trans isomer	2.056	2.2567	2.1229	14	164	63.9	7.8	9.0	0.45
cis isomer	2.056	2.2564	2.1228	20	182	74.0	7.8	10.5	0.55
$Cu(L\text{-}LysH)_2^{2+}$									
trans isomer	2.055	2.2552	2.1217	11	166	63.6	8.0	8.7	0.46
cis isomer	2.055	2.2572	2.1224	20	183	74.2	8.0	10.7	0.54
$Cu(L\text{-}Pro)_2$									
trans isomer	2.057	2.2523	2.1221	15	161	63.6	5.5	9.3	0.49
cis isomer	2.057	2.2511	2.1217	20	183	74.5	5.5	10.7	0.51
$Cu(Sar)_2$									
trans isomer	2.057	2.265	2.1264	15	158	63.7	4.4	9.0	0.74
cis isomer	2.057	2.274	2.1281	20	176	74.2	4.4	9.5	0.26

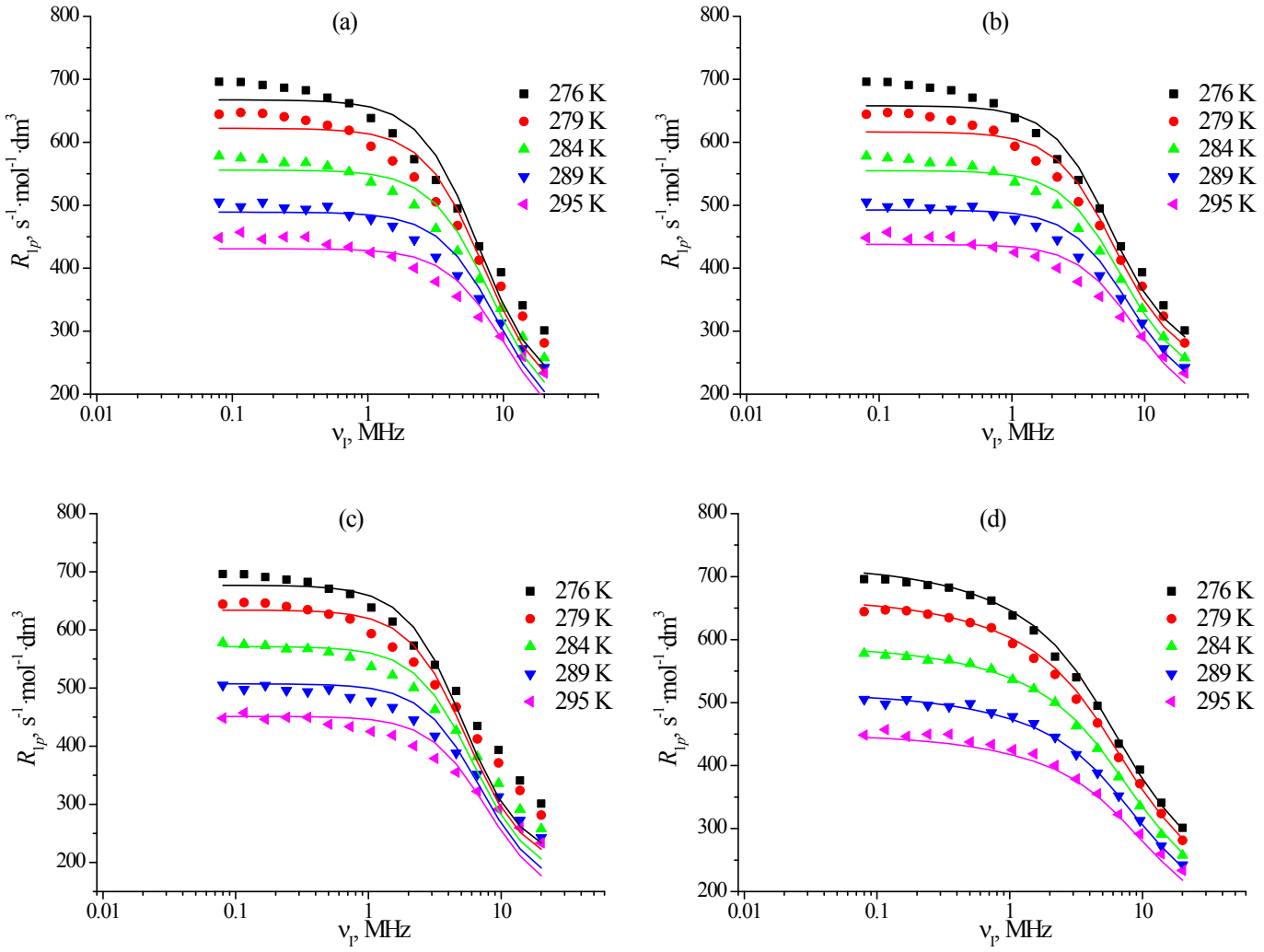

Fig. 2S Experimental (points) NMRD profiles for the $Cu(Gly)_2$ aqueous solution and simulated (lines) by different models: a) model 1: inner sphere, b) model 2: inner sphere + second sphere, c) model 3: inner sphere + rotational outer sphere, d) model 4: inner sphere + translational outer sphere (d = 3.03 Å).

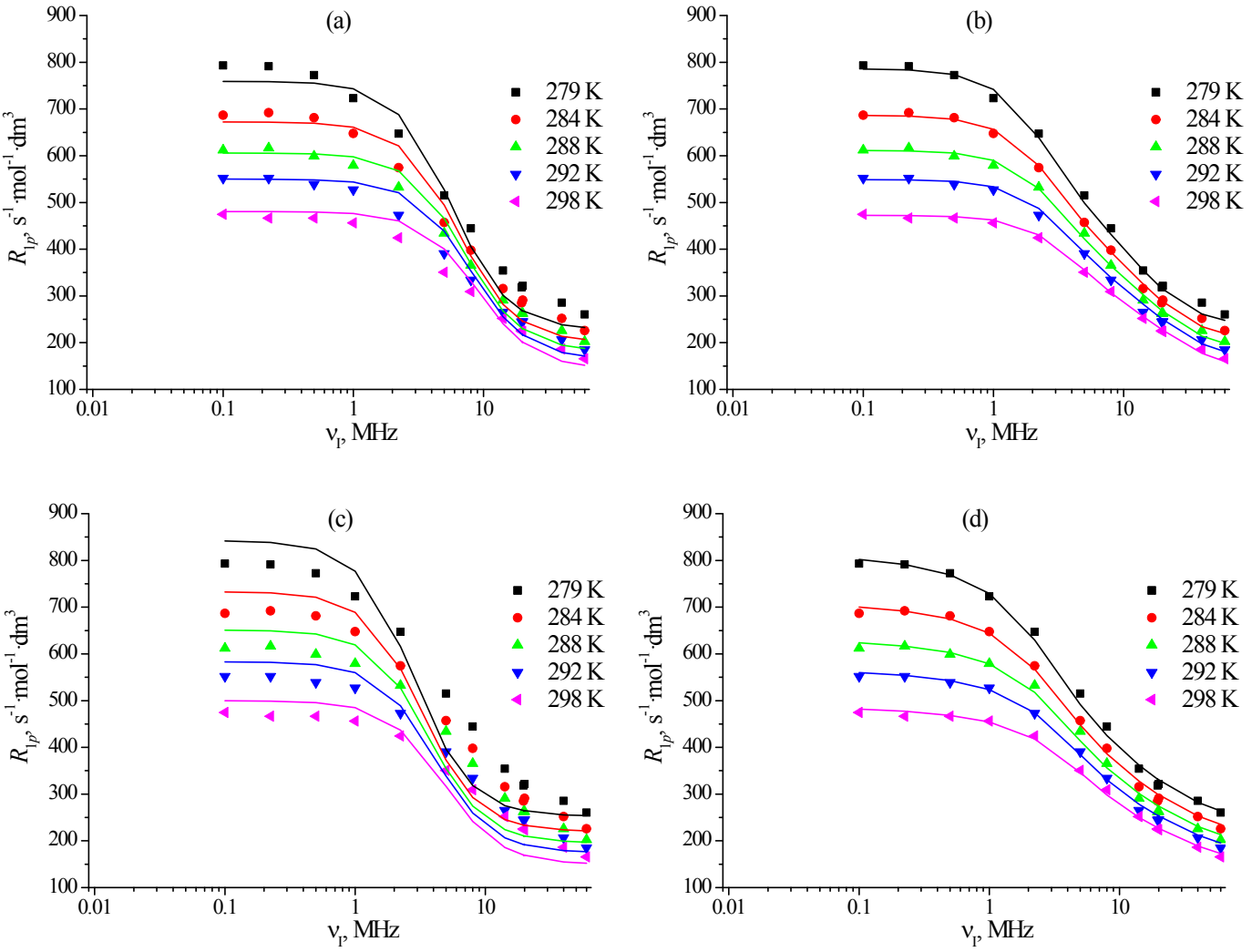

Fig. 3S Experimental (points) NMRD profiles for the Cu(*L*-Glu)$_2^{2-}$ aqueous solution and simulated (lines) by different models: a) model 1: inner sphere, b) model 2: inner sphere + second sphere, c) model 3: inner sphere + rotational outer sphere, d) model 4: inner sphere + translational outer-sphere (d = 2.98 Å).

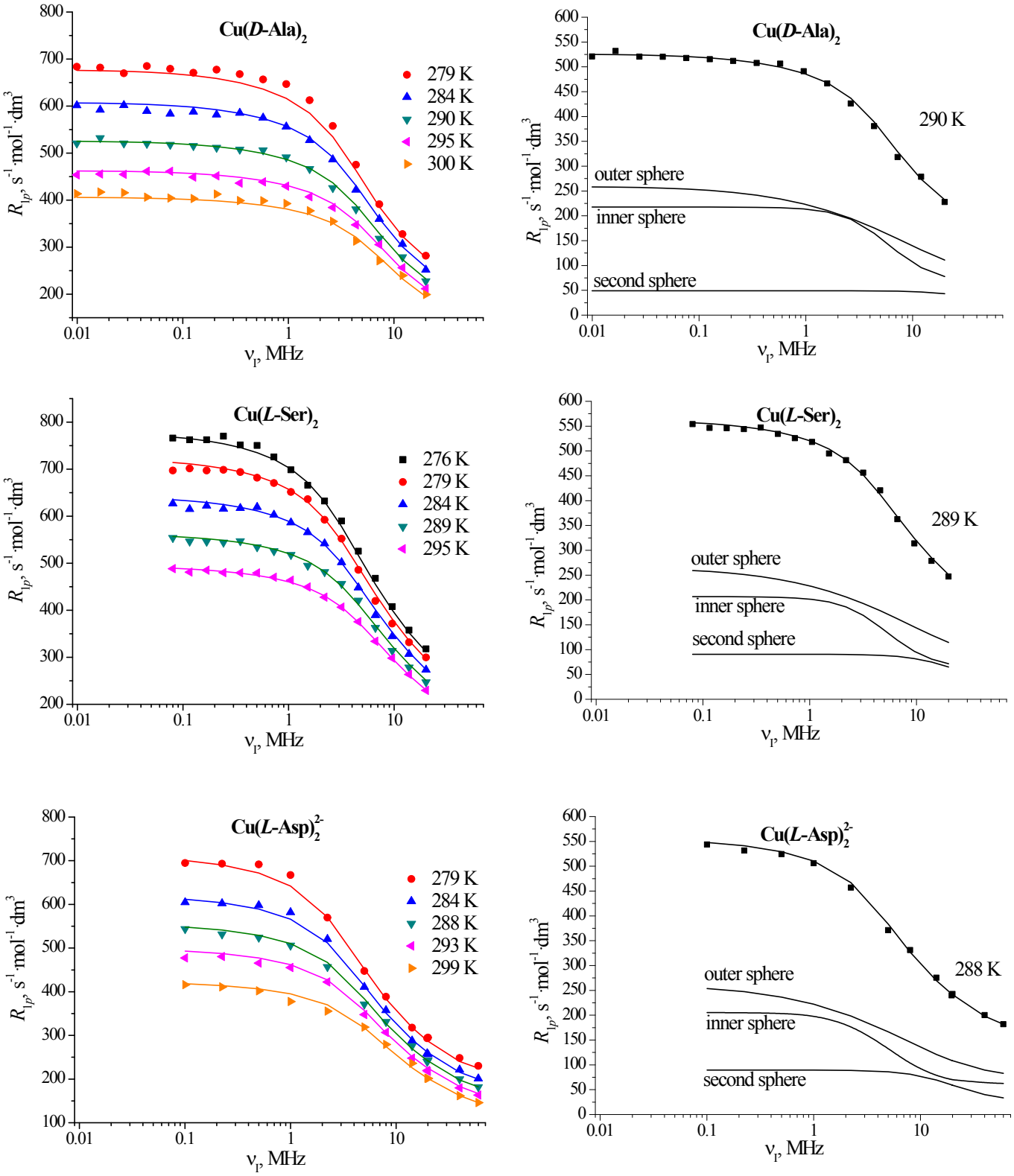

Fig. 4S Left column: experimental NMRD profiles (points) and their best simulations (lines); right column: experimental (points) and fitted (lines) NMRD profiles with different contributions. The abscissa is $\nu_I = \omega_I/2\pi$. $R_{1p} = T_{1p}^{-1}/C_M$ is the molar relaxivity, where C_M is the metal concentration.

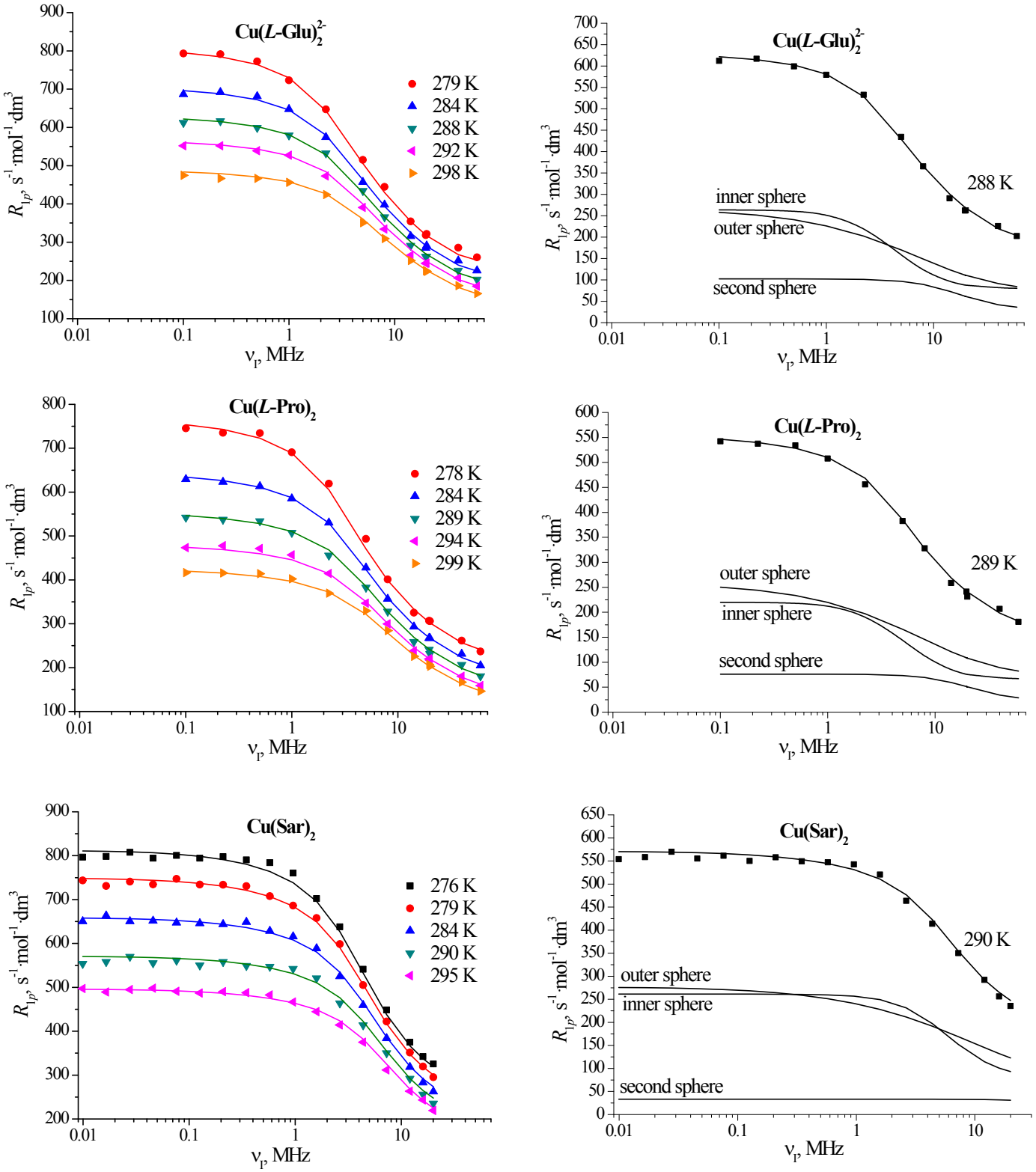

Fig. 5S Left column: experimental NMRD profiles (points) and their best simulations (lines); right column: experimental (points) and fitted (lines) NMRD profiles with different contributions. The abscissa is $\nu_I = \omega_I/2\pi$. $R_{1p} = T_{1p}^{-1}/C_M$ is the molar relaxivity, where C_M is the metal concentration.

cis-Cu(Gly)$_2$·1H$_2$O
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trans-Cu(Gly)$_2$·1H$_2$O
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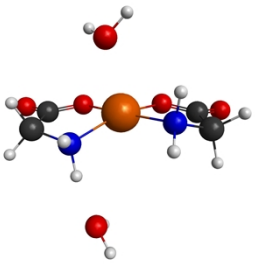

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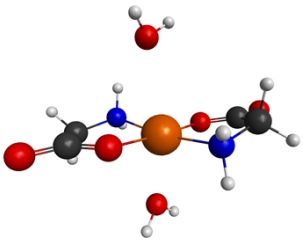

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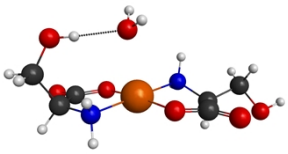

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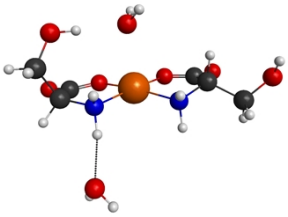

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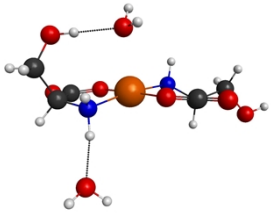

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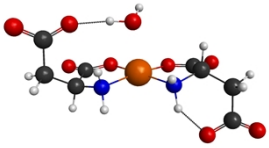

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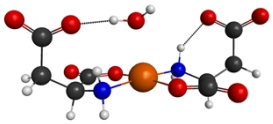

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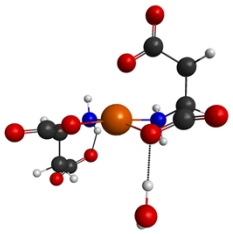

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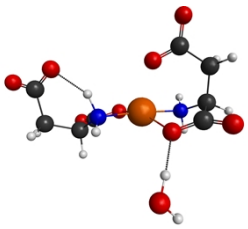

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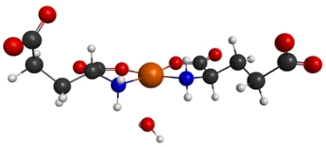

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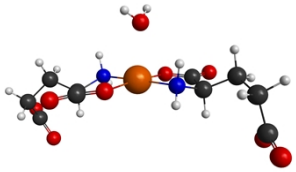

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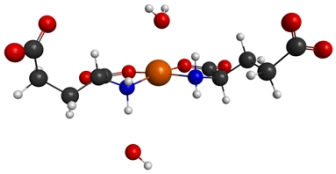

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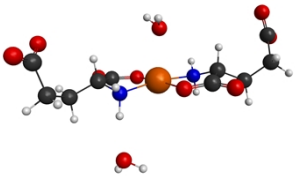

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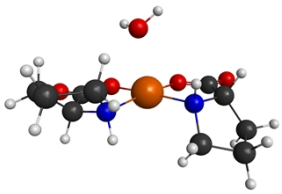

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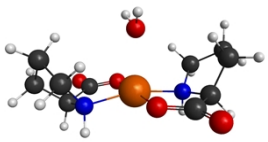

trans-Cu(*L*-Pro)$_2$·1H$_2$O
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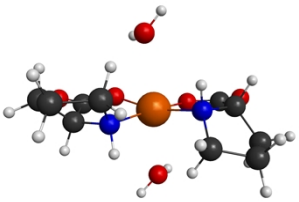

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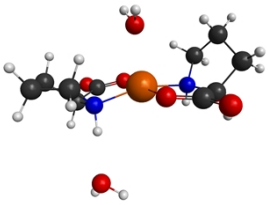

trans-Cu(*L*-Pro)$_2$·2H$_2$O
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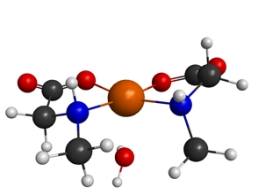
Fig. 6S Structures of some copper(II) *bis*-complexes with amino acids optimized in GAMESS program package at B3LYP/TZVP level using C-PCM model to account solvent effects.



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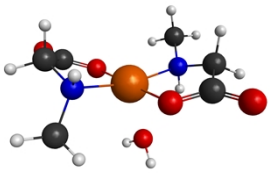

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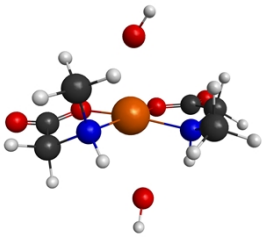

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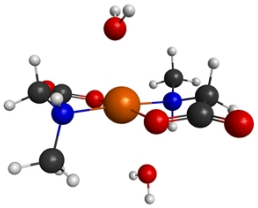

trans-Cu(Sar)$_2$·2H$_2$O
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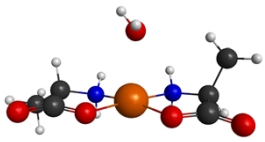

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trans-Cu(*L*-Ala)$_2$·1H$_2$O
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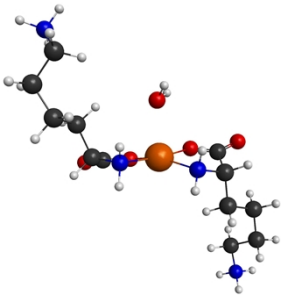

cis-Cu(*L*-LysH)$_2^{2+}$·1H$_2$O
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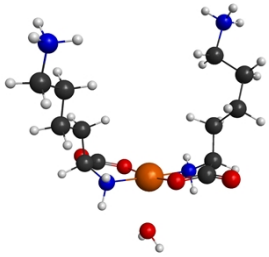

trans-Cu(*L*-LysH)$_2^{2+}$·1H$_2$O
E = -2710.5728 a.u.

Fig. 6S (continuation) Structures of some copper(II) *bis*-complexes with amino acids optimized in GAMESS program package at B3LYP/TZVP level using C-PCM model to account solvent effects.

Table 2S Distances between copper(II) and water molecules in optimized structures (r_{O1w}, r_{O2w}) and electric dipole moments of complexes (*D*)

Complex	r_{O1w} / Å	r_{O2w} / Å	*D* / Debye
cis-Cu(Gly)$_2$·1H$_2$O	2.48		0.88
trans- Cu(Gly)$_2$·1H$_2$O	2.43		0.13
cis-Cu(Gly)$_2$·2H$_2$O	2.44	3.77	0.78
trans- Cu(Gly)$_2$·2H$_2$O	2.46	2.99	0.10
cis-Cu(*L*-Ser)$_2$·1H$_2$O	2.72		1.00
trans- Cu(*L*-Ser)$_2$·1H$_2$O	2.62		0.19
cis-Cu(*L*-Ser)$_2$·2H$_2$O	2.62	4.13	0.98
trans- Cu(*L*-Ser)$_2$·2H$_2$O	2.62	4.14	0.24
cis-Cu(*L*-Asp)$_2^{2-}$·1H$_2$O	2.47		0.45*
trans-Cu(*L*-Asp)$_2^{2-}$·1H$_2$O	2.43		0.75*
cis-Cu(*L*-Asp)$_2^{2-}$·1H$_2$O (-O$_{ax}$)	4.14		0.57*
trans-Cu(*L*-Asp)$_2^{2-}$·1H$_2$O (-O$_{ax}$)	4.30		0.89*
cis-Cu(*L*-Glu)$_2^{2-}$·1H$_2$O	2.54		0.76*
trans-Cu(*L*-Glu)$_2^{2-}$·1H$_2$O	2.51		0.91*
cis-Cu(*L*-Glu)$_2^{2-}$·2H$_2$O	2.55	3.91	0.60*
trans-Cu(*L*-Glu)$_2^{2-}$·2H$_2$O	2.47	4.03	0.59*
cis-Cu(*L*-Pro)$_2$·1H$_2$O	2.48		0.81
trans-Cu(*L*- Pro)$_2$·1H$_2$O	2.43		0.07
cis-Cu(*L*- Pro)$_2$·2H$_2$O	2.55	2.75	0.70
trans-Cu(*L*- Pro)$_2$·2H$_2$O	2.43	4.09	0.09
cis-Cu(Sar)$_2$·1H$_2$O	2.46		0.89
trans-Cu(Sar)$_2$·1H$_2$O	2.45		0.06
cis-Cu(Sar)$_2$·2H$_2$O	2.55	2.85	0.83
trans-Cu(Sar)$_2$·2H$_2$O	2.52	3.11	0.05
cis-Cu(*L*-Ala)$_2$·1H$_2$O	2.54		0.91
trans- Cu(*L*-Ala)$_2$·1H$_2$O	2.46		0.05
cis-Cu(*L*-LysH)$_2^{2+}$·1H$_2$O	2.48		0.78*
trans-Cu(*L*-LysH)$_2^{2+}$·1H$_2$O	2.44		1.37*

* In the case of Cu(*L*-Asp)$_2^{2-}$, Cu(*L*-Glu)$_2^{2-}$, and Cu(*L*-LysH)$_2^{2+}$ the calculated dipole moments are depend on arrangement of uncoordinated charged groups of ligands. So their exact calculations in this model (with only 1 or 2 H$_2$O) were not possible.

Table 3S Atomic coordinates for the $Cu(Gly)_2 \cdot 44H_2O$ complex optimized at the PBE/L2 level (L2 basis set: H {8s4p2d}/[3s2p1d]; C, N, O {12s8p4d2f}/[4s3p2d1f]; Cu {23s18p13d2f}/[6s5p3d1f])

Atom	x / Å	y / Å	z / Å
Cu	6.47646750	0.98078498	-0.64326375
N	6.79481377	2.56017559	-1.88098785
H	7.10954725	2.20925236	-2.79821376
C	7.80309834	3.44688593	-1.26445331
H	8.75970783	3.33909615	-1.79367457
H	7.49866529	4.50244121	-1.31374714
C	8.07952777	3.06857409	0.19060637
O	8.79671867	3.82065840	0.90468325
O	7.59824692	1.96604657	0.61391590
O	7.27344112	-0.24903912	3.03507443
H	6.42656601	-0.00687736	3.49651386
H	7.03270276	-0.40128431	2.08706296
C	5.07736539	-1.45587088	-1.18114355
N	5.56427505	-0.28103610	-1.92429637
H	5.03178953	-2.35763453	-1.80598228
H	4.06397139	-1.26193684	-0.79800121
C	5.97576013	-1.70329695	0.03426314
O	6.03756891	-2.83945059	0.56729041
O	6.61935774	-0.68187538	0.46006943
H	6.39576034	-0.58816336	-2.45932065
H	4.86999026	0.13748546	-2.56639549
O	4.49866869	1.86529955	0.44653495
H	4.72708508	2.41187943	1.24656344
H	3.73093016	1.28185654	0.67871871
H	5.89471732	3.05828155	-1.97689069
O	8.94715911	1.83020697	3.37553068
H	8.32020818	1.09940001	3.09661581
H	8.86537988	2.50296698	2.66579313
O	2.28523524	0.23429659	0.83714891
H	2.38797444	-0.70849545	1.16178009
H	1.84649595	0.18998985	-0.04721997
O	6.19056689	-3.57127168	3.34227869
H	7.06142001	-3.37717332	3.72929790
H	6.26192960	-3.26670775	2.41086134
O	9.21868343	-2.20656239	3.22079007
H	8.46885801	-1.56304465	3.25965047
H	9.98803425	-1.59436295	3.05279299
O	11.42111736	2.98116761	-0.24580455
H	11.26755811	2.03425371	-0.04737463
H	10.66307343	3.43870592	0.16871750
O	5.08455315	5.92192214	0.46986623
H	6.07031627	6.11630412	0.52170951
H	4.64328960	6.75460768	0.69737032
O	4.22201075	3.88754649	-1.33261136
H	4.40360569	4.71139786	-0.82546259
H	4.21654205	3.16675838	-0.64097268
O	1.15416283	0.33611889	-1.72608345
H	1.45970618	-0.24380588	-2.47730434
H	0.18630529	0.27380852	-1.73341504
O	3.30906742	2.42889175	4.06736779
H	2.42115603	2.10382125	3.76269538
H	3.64793896	2.97477967	3.31839808
O	4.90911873	3.79627540	2.29721040
H	5.35496678	4.00843368	3.17038987
H	4.89895361	4.62758113	1.76757687
O	9.90218263	-2.17916338	-0.80020130
H	10.30906259	-2.78043662	-1.48194743
H	9.55116310	-2.77466876	-0.05966999
O	8.10567793	-1.32249624	-2.54008802

H	8.63052225	-1.71607884	-1.77597942
H	8.60297095	-0.44525851	-2.63002806
O	3.89573867	1.08050685	-4.00435946
H	3.29894677	1.80031011	-3.62061273
H	3.26208949	0.35190821	-4.20546773
O	5.10998377	0.47924363	4.55049321
H	5.73782760	0.90599785	5.17023684
H	4.43900575	1.19517034	4.32915720
O	8.85120743	-3.70448655	1.06350736
H	9.02808277	-3.17540332	1.91536254
H	7.89866994	-3.56792518	0.88786791
O	9.43216084	0.92649980	-2.30772253
H	10.13607188	0.73973492	-1.64079378
H	9.87712020	1.29738214	-3.11618740
O	2.57063190	-2.26451999	1.83190542
H	3.17623472	-2.17058978	2.66985704
H	1.73369753	-2.59943727	2.19170288
O	4.00723340	-2.08223648	3.97340572
H	4.82663965	-2.63900392	3.85602039
H	4.34509928	-1.20037968	4.25553203
O	3.66237335	-3.02950173	-4.34247186
H	3.90486402	-3.67744024	-3.62765570
H	4.48992893	-2.79872215	-4.81662021
O	2.06059332	-1.03333233	-3.93636747
H	2.67967401	-1.84287435	-4.03278555
H	1.40775840	-1.13202117	-4.64660389
O	4.33138788	-4.81863066	-2.37061448
H	4.00917940	-5.71049558	-2.57596488
H	3.99990025	-4.62495822	-1.43047100
O	3.79397152	-4.33125135	0.14959755
H	3.19158337	-3.70258679	0.60472214
H	4.68023559	-3.93220040	0.34283326
O	11.24983637	0.08442341	-0.26727624
H	10.77641714	-0.79114127	-0.38528547
H	12.07625980	-0.01032296	-0.80808921
O	7.71727795	6.30908859	0.75069078
H	8.24448267	6.83586192	0.13136972
H	8.20698801	5.44317557	0.84211261
O	0.97518105	1.45176095	2.96001083
H	1.37283692	1.00334832	2.16854486
H	0.62671892	0.72741082	3.50241584
O	8.20922329	-3.29924928	-4.25184971
H	7.40151614	-3.30616442	-4.81224005
H	8.08553193	-2.54802634	-3.58545619
O	9.59121285	-5.63408262	-1.08265159
H	8.68744540	-5.67440395	-1.48775181
H	9.44958557	-5.16913432	-0.23204400
O	10.70535020	-3.89254803	-2.79838417
H	10.42825821	-4.64356308	-2.18121255
H	9.97108174	-3.84813951	-3.44366633
O	7.68138470	1.42838111	-4.66859819
H	6.96382052	1.83028364	-5.23941867
H	8.52238831	1.92397307	-4.79269087
O	5.44972398	2.10355417	-5.97910416
H	5.18014082	3.02832268	-6.08675502
H	4.81623082	1.73171717	-5.29918844
O	10.43437713	2.06974491	-4.58532871
H	11.19805198	2.41521142	-4.02130894
H	10.80423292	1.31835691	-5.10005468
O	8.29370035	-0.90591047	-5.90291343
H	8.04172187	-0.07452530	-5.39115814
H	8.48099368	-1.59870545	-5.22958578
O	12.46298164	-1.88056321	-3.86926666

H	11.95070477	-2.62941091	-3.48773092
H	11.88976448	-1.47881574	-4.55867085
O	11.00304574	-0.40385608	-5.90489363
H	11.44308268	-0.44777950	-6.76804662
H	10.04230274	-0.60227170	-6.08005568
O	11.03322613	-0.17195362	2.69240927
H	11.19605388	-0.05542072	1.73188168
H	10.47600788	0.59833489	2.94009829
O	7.24248402	-5.47963880	-2.58000218
H	7.55654835	-4.76456145	-3.17545043
H	6.32924099	-5.21638987	-2.34277426
O	12.38257344	2.69342393	-2.87025524
H	12.78907472	1.81359468	-2.69986199
H	12.00675806	2.94018537	-1.98758649
O	13.23341838	0.01103984	-2.18149157
H	14.16721633	-0.16067216	-1.98489602
H	12.95152851	-0.72540688	-2.81807181
O	6.03365970	-2.55108574	-5.94542268
H	5.91128032	-2.98416679	-6.80486690
H	6.67118846	-1.80886974	-6.11727539
O	2.22900059	2.84939312	-2.89667421
H	2.82607180	3.36492249	-2.29437015
H	1.77836344	2.19903136	-2.32012418
O	7.33059066	2.18831184	5.50232962
H	7.99805249	2.12984354	4.74945918
H	7.86263254	2.23571774	6.31147209
O	5.60689938	4.23189761	4.84820541
H	4.75351952	3.85693065	5.13368219
H	6.27315562	3.55982088	5.14800963

Table 4S Atomic coordinates for the *cis*-$Cu(Gly)_2 \cdot 1H_2O$ structure optimized at the B3LYP/TZVP level using C-PCM model

Atom	x / Å	y / Å	z / Å
Cu	6.5057009867	0.5627768302	0.3076671575
N	8.3283680746	1.1693522443	-0.4151607084
H	8.9114788593	0.3508898163	-0.5679763296
C	8.9528484455	2.0642178728	0.5928805826
H	10.0307768383	1.9156021433	0.6492488314
H	8.7775837311	3.1000718067	0.2998824307
C	8.3305330706	1.8677237113	1.9810092786
O	8.8840453068	2.3644801844	2.9641977328
O	7.2219594037	1.2101486693	2.0180920342
C	4.6882892732	-1.2712065538	-0.9929263696
N	5.7787970312	-0.3395112324	-1.3819927277
H	5.0678748349	-2.2930739432	-1.0102951477
H	3.8523859210	-1.2199584778	-1.6903923177
C	4.1820659139	-0.9899506815	0.4254591617
O	3.1644630405	-1.5663665592	0.8171360945
O	4.8796706091	-0.1697311996	1.1336008243
H	6.4960046145	-0.8349312840	-1.9012933524
H	5.4228165197	0.3790689620	-2.0059042040
O	5.5775909809	2.8241228259	-0.1105035640
H	4.6689481363	2.9486342876	-0.4097160613
H	5.6225725900	3.2813917549	0.7379267019
H	8.2532258182	1.6402488226	-1.3119400477

Table 5S Atomic coordinates for the *trans*-$Cu(Gly)_2 \cdot 1H_2O$ structure optimized at the B3LYP/TZVP level using C-PCM model

Atom	x / Å	y / Å	z / Å
Cu	4.8526688037	0.2100747857	0.8406303127
N	5.0800297677	0.5104572811	2.8435795538
C	3.6729776690	-1.1675407927	-1.3948441482
N	4.8304225908	-0.2762227321	-1.1422314973
H	3.9115986197	-1.9518477106	-2.1132884445
H	2.8544767741	-0.5800891804	-1.8128747656
C	3.1623459055	-1.8050985305	-0.0953784672
O	2.3517591216	-2.7310850341	-0.1581142290
O	3.6041740469	-1.2931818268	1.0044060195
H	5.7017043633	-0.7638587972	-1.3316055506
H	4.8168534711	0.5357976459	-1.7510211971
O	3.1748224461	1.9700251247	0.7639878119
H	3.4404041895	2.8065519134	0.3647351430
H	2.2393637363	1.8608821619	0.5586897683
H	4.2860466175	1.0925438802	3.0960423443
H	5.0133029728	-0.3391832835	3.3939700440
C	6.3545258315	1.2253174863	3.0813861432
C	6.8493348482	1.9175515965	1.8045929963
O	6.2722791204	1.5666382522	0.7046535394
O	7.7674936006	2.7368795216	1.8814780069
H	6.2718851581	1.9561828149	3.8853529613
H	7.1155303457	0.5012054236	3.3758536549

Table 6S Atomic coordinates for the *cis*-$Cu(Gly)_2 \cdot 2H_2O$ structure optimized at the B3LYP/TZVP level using C-PCM model

Atom	x / Å	y / Å	z / Å
Cu	-0.3977358775	0.2538934320	0.0343404709
N	1.5849487461	0.3892316841	-0.4025477697
H	1.9397503880	-0.5546060071	-0.2169840348
C	2.2111313501	1.3722828885	0.5104338004
H	3.2151652372	1.0674653705	0.8073852889
H	2.2956293828	2.3333968425	0.0009631523
C	1.3502390035	1.5864319335	1.7615979869
O	1.8166847604	2.2056418297	2.7212664893
O	0.1488044077	1.1171276881	1.7153140353
O	2.2713003578	-2.3807417410	0.3685141316
H	1.9738801285	-2.7644454493	1.2011819233
H	2.4022138006	-3.1241268425	-0.2309436585
C	-2.2092615037	-1.6281553113	-1.2218100694
N	-1.1146529816	-0.7118849682	-1.6325312184
H	-1.8114718839	-2.6406005632	-1.1422440633
H	-3.0151467830	-1.6470348309	-1.9557584751
C	-2.7729880860	-1.2447248596	0.1503956292
O	-3.8058381506	-1.7923254982	0.5457583256
O	-2.0955035349	-0.3785692121	0.8198300786
H	-0.4193752992	-1.2163280212	-2.1716017462
H	-1.4763874550	0.0121038416	-2.2471005632
O	-1.0150893882	2.4653437584	-0.8025535903
H	-1.8157978501	2.6999684394	-1.2866682285
H	-0.9967712629	3.0569862856	-0.0411316023
H	1.7807021991	0.6079154831	-1.3739544130

Table 7S Atomic coordinates for the *trans*-$Cu(Gly)_2 \cdot 2H_2O$ structure optimized at the B3LYP/TZVP level using C-PCM model

Atom	x / Å	y / Å	z / Å
Cu	0.1365438763	-0.1409301973	-0.1025088699
N	0.0696799217	0.4242123545	1.8495175281
O	1.9092395864	-1.7952591139	0.3019437340
H	1.7648436886	-2.7482687726	0.3280396785
H	2.8110482263	-1.6716689873	-0.0149130714
C	-1.3564648110	-1.1729757823	-2.3317154718
N	-0.0594313196	-0.4919604371	-2.1033720343
H	-1.2996822924	-1.9024870861	-3.1390174945
H	-2.0995906149	-0.4259208113	-2.6149695093
C	-1.8598847502	-1.8561129188	-1.0522995763
O	-2.7839867717	-2.6708062382	-1.1319475052
O	-1.2883622456	-1.5006771090	0.0455767171
H	0.7122301718	-1.1010985247	-2.3616399183
H	0.0260424086	0.3432492112	-2.6739819580
O	-1.9831764648	1.9211236120	0.3093840433
H	-1.9437373681	2.8013048549	-0.0824891755
H	-2.9005413864	1.6405077358	0.2136234752
H	-0.7606475669	1.0138897275	1.8523241653
H	-0.0670340937	-0.3284057962	2.5149705125
C	1.2859915287	1.2081912328	2.1468992732
C	1.9123267312	1.7756467414	0.8654894474
O	1.4788302820	1.2877308335	-0.2467881139
O	2.8000940114	2.6285803648	0.9543790189
H	1.0931279762	2.0234885557	2.8456778473
H	2.0271412760	0.5499465508	2.6029172576